LCF Seminar Series

Thermodynamics of magnetic systems from first principles: WL-LSMS

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January 28, 2010

1:00 p.m., Building 4500N, Weinberg Auditorium

Abstract:

Calculating the thermodynamics of nanoscale systems presents challenges in the simultaneous treatment of the electronic structure, which determines the interactions between atoms, and the statistical fluctuations that become ever more important at shorter length scales. Density Functional Calculations have proven to be a useful tool to study the ground state of many materials. For finite temperatures the situation is less ideal an one is often forced to rely on models with parameters either fitted to first principles or experimental results. This approach is especially unsatisfactory in inhomogeneous systems, nano particles or other systems where the model parameters should vary significantly from one site to another.
Here we present a highly scalable method that combines ab initio electronic structure techniques, we use the Locally Self-Consitent Multiple Scattering (LSMS) technique, with the Wang-Landau (WL) algorithm to compute free energies and other thermodynamic properties of nanoscale systems. The combined WL-LSMS code is targeted to the study of magnetic systems that have anywhere from about one hundred to a few thousand atoms. The combined code shows superb scaling behavior on massively parallel computers, having achieved 1.83 PFlops on the jaguar system at Oak Ridge.

Bio:
Dr. Eisenbach is a computational scientist at the National Center for Computational Sciences. His expertise lies in first principles calculations for magnetic materials and large scale scientific computing. He is the key developer of the relativistic linear scaling multiple scattering code (rel-LSMS) and the Wang-Landau LSMS method for first principles finite temperature calculations of magnetic systems. He was a co-recipient of the SC'08 Gordon-Bell price for his contribution to the DCA++ code development.

Host: Ricky Kendall, kendallra@ornl.gov (865-576-6905)